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Floating Point Cowell (Second-Sum), Runge-Kutta
Integration of Second-Order Ordinary Differential Equations
(Subroutine ASC DEQ4)

Prepared by JAMES F. HOLT
Electronics Division

May 1968

El Segundo Technical Operations
AEROSPACE CORPORATION

Prepared for SPACE AND MISSILE SYSTEMS ORGANIZATION
AIR FORCE SYSTEMS COMMAND
LOS ANGELES AIR FORCE STATION
Los Angeles, California

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FLOATING POINT COWELL (SECOND-SUM), RUNGE-KUTTA
INTEGRATION OF SECOND-ORDER ORDINARY
DIFFERENTIAL EQUATIONS
(SUBROUTINE ASC DEQ4)

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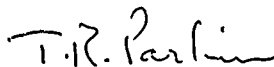
FOREWORD

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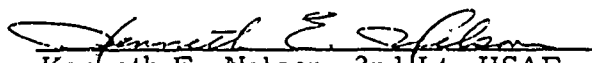
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Kenneth E. Nelson, 2nd Lt, USAF
Project Officer

ABSTRACT

ASC DEQ4 is a floating point subroutine, written in FORTRAN IV source language, which integrates numerically a set of N simultaneous second-order ordinary differential equations in which first derivatives may or may not appear [i.e., $y_i'' = f(t, y_i, y_i')$ or $y_i'' = f(t, y_i)$, $i = 1, 2, \dots, N$]. If the N equations can be separated into two groups (IB and N-IB) such that the first IB equations are not dependent on the final N-IB equations (e. g., variational equations) then DEQ4 has the capability of integrating the final N-IB equations at a larger step size than the first IB equations, thus saving $2(R-1)(N-IB)$ derivatives per integration step. This subroutine obsoletes subroutine DEQ2 with the following improvements: better accuracy controls, new starting procedure, improved halving and doubling procedure, reduction in computing time, and reduction in core storage requirements (10N less).

The subroutine is restricted in that it contains 20 digit octal constants (real constants) for the CDC 3000 series machines.

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SECTION I

INTRODUCTION

A. PURPOSE

The purpose of ASC DEQ4 is to integrate numerically a set of N simultaneous second-order ordinary differential equations in which first derivatives may or may not appear [i. e., $y_i'' = f(t, y_i, y_i')$ or $y_i'' = f(t, y_i)$ $i = 1, 2, \dots, N$]. If the N equations can be separated into two groups (IB and N-IB) such that the first IB equations are not dependent on the final N-IB equations, then DEQ4 has the capability of integrating the final N-IB equations at a larger step size (ratio = $R = 2^K$, $K \geq 1$) than the first IB equations. This will save $2(R-1)(N-IB)$ derivatives per integration step when operating in the Cowell mode.

B. RESTRICTIONS

The restrictions associated with the use of ASC DEQ4 are as follows:

1. No internal checks are made for overflow or underflow.
2. The user must provide an auxiliary subroutine (DAUX) which evaluates the second-order derivatives and the name of the auxiliary subroutine must be defined as an argument in the calling sequence and also through the use of the EXTERNAL statement in the main program (i. e., EXTERNAL DAUX).
3. If the two-group, multi-step mode is used, then DAUX should be programmed to skip the evaluation of the final N-IB derivatives when TEST is negative. (See IB, TEST, and VMIN in Section II-A for restrictions on the use of the two-group, multi-step mode.
4. Initial conditions must be stored prior to entering the program.
5. ASC DEQ4 is a single precision subroutine written in Fortran IV Source Language.
6. The subroutine contains 20 digit octal constants (real constants) for the CDC 6000 series machines.

C. METHOD

A fourth-order Runge-Kutta method¹ is used to start the integration and to halve the step size during integration. A Cowell "second-sum" method based on eighth differences is used to continue the integration. Doubling is accomplished in the Cowell mode through the accumulation of alternate steps. Truncation error can be controlled by choosing an appropriate step size, and by using the variable step size mode of operation. DEQ4 has an automatic restart procedure which works as follows:

After eight Runge-Kutta steps ($h = H/IR$), an attempt is made to integrate in the Cowell mode ($h = H/IR$). If the error criterion (see ER in Section II-A) cannot be satisfied for the first IB equations, the initial conditions (i. e., t_0 , y'_{i0} , and y''_{i0}) are restored, the step size is reduced to $h = h/2*IR$, and the integration is restarted. This procedure continues until the error criterion is satisfied, or until $h < HMIN$. For the latter, the subroutine sets TEST = 13 and exits to the user.

Note: Either $I2 < 0$, or $HMIN = HMAX$ nullifies the restart procedure as well as the halving procedure.

¹J. B. Scarborough, Numerical Mathematical Analysis, Third Edition, John Hopkins Press, Baltimore (1955) pp. 301-302.

SECTION II

PROGRAM USAGE

A. CALLING SEQUENCE¹

CALL DEQ4(N, I1, I2, IA, IB, IR, ER, HMIN, HMAX, YMIN,
DAUX, TEST, IDH, NTRY, JHH, JHD, VMIN, VMAX, T,
H, Y, YP, Y2P, T1, T2, T3, T4, T5, T6, T7, F2P, F1P,
DLT1, DLT2, DLT3, DLT4, DLT5, DLT6, DLT7, DLT8)

The nomenclature is as follows:

- N the number of equations.
- I1 an option, so that if
 $I1 \geq 0$, 1st derivatives are present in the evaluation of
 the second derivatives, $[y_i'' = f(t, y_i, y_i')]$.
 $I1 < 0$, 1st derivatives are missing in the evaluation of
 the second derivatives, $[y_i'' = f(t, y_i)]$.
- I2 an option, so that if
 $I2 \geq 0$, variable step size mode of operation is used.
 $I2 < 0$, fixed step size mode of operation is used.
 (Note: For $I2 < 0$, $h = H/IR$ for all steps.)
- IA an indicator switch to the user during exit to DAUX.
 $IA = -1$ for first (1, 2, 3 if Runge-Kutta) pass through DAUX.
 $IA = +1$ for final (4th if Runge-Kutta) pass through DAUX.
 This applies for each integration step. In the Cowell mode,
 $IA = -1$ when the derivatives of the predictor are being
 asked for, and $IA = +1$ when the derivatives of the corrector
 are being asked for.
- IB Only the first IB ($\leq N$) equations are tested to determine whether
 it is necessary to halve or possible to double the step size or to
 proceed with a Cowell integration step. (See Section I-A and
 Section II-C for an additional use of IB.)

¹ See NTRY and Section II-B

IR For a given step-size H, the initial step size for both Runge-Kutta and Cowell will be $h = H/IR$. If halving is required, the current step-size h is reduced to $h = h/(2*IR)$ for all N equations, and the integration procedure returns to the Runge-Kutta mode. (Usually $IR = 8$ or 16 ; if $IR = 0$, DEQ4 sets $IR = 16$.)

ER The user should set $ER = 1E - S$ (i. e. , 10^{-S}), where S is the approximate number of significant figures desired. If $ER = 0$, DEQ4 sets $ER = 1E - 11$. (User should test for best ER.) In general, $ER \leq 1E - 11$ is recommended.

HMIN the minimum absolute value of the step size allowed when halving is required. During the starting procedure (see Section I-C), if halving is required and $h/(2*IR) < HMIN$, the integration is terminated with $TEST = 13$; otherwise, the integration is continued in the Cowell mode with the current step-size h (i. e. , halving is not permitted). If $HMIN = HMAX$, all halving is suppressed during the entire integration procedure. If $HMIN = 0$, DEQ4 sets $HMIN = 1E - 5$. Only the first IB equations are tested for halving.

HMAX the maximum absolute value of the step size allowed for the first IB equations. The final N-IB equations may be integrated at a larger step size when operating in the two-group, multi-step integration mode (see Section I-A). If $HMAX = 0$, DEQ4 sets $HMAX = 1$. A value of $HMAX \leq 16$ is recommended for most problems.

YMIN the minimum absolute value allowed for y_i for the relative error test during the halving and doubling procedure. YMIN prevents unnecessary halving for $y_i \approx 0$. If $YMIN = 0$, DEQ4 sets $YMIN = 1$. (User should supply YMIN).

Note: For the more difficult problems, it may be necessary for the user to modify the subroutine and make YMIN a vector of dimension IB -- thus allowing a different YMIN for the first IB equations.

DAUX the location of the entry point of an external subroutine (supplied by the user) which evaluates and stores (see Y2P) the second-order derivatives y_i'' . DAUX must be defined by the user through the use of the EXTERNAL statement in the main program, and COMMON must be used as a means of data linkage. CALL DAUX is used by DEQ4 to enter DAUX. If the two-group, multi-step mode is used, then DAUX should be programmed to skip the evaluation of the final N-IB derivatives when TEST is negative.

TEST

has the following multiple uses:

Initially (i. e. , prior to NTRY = 1), the user must set:

TEST = +1., to integrate the N equations at the same step size.

TEST \geq +2., to use the two-group, multi-step mode. The maximum ratio of the step sizes for the two groups will be $R_{MAX} = 2^{**}(TEST - 1)$. Recommend TEST \leq 5.

After each integration step (NTRY = 2) DEQ4 will set:

TEST = +1., if the integration was a Runge-Kutta step (i. e. , during starting procedure, or halving procedure if JHH = 1).

TEST = +2., if the integration has been restarted during the initial starting procedure. Indicates $h = h/(2*IR)$ and Runge-Kutta step.

TEST = +3., if the step size has been reduced [$h = h/(2*IR)$], and the integration has been returned to a previous step during the halving procedure (possible only if JHH = 3).

TEST = -1., if the integration was a Cowell step.

During the starting procedure (see Section I-C):

TEST = +13., if the integration has been terminated during the restarting procedure. Indicates programming error, or ER, H, or HMIN too restrictive.

During transfers to DAUX (also, see IA and DAUX):

TEST = -1., when the first IB equations are being integrated (at a smaller step-size) in the multi-step Cowell mode.

TEST = +1., when the N equations are being integrated in the Runge-Kutta or Cowell mode.

IDH

an indicator switch to the user after each integration step.

IDH = 1, if the step size has not changed

IDH = 2, if the step size of all N equations has been reduced to $h = h/(2*IR)$ where h is the current step size of the first IB equations.

IDH = 3, if the step size of all N equations has been doubled.

IDH = 4, if the step size of the final N-IB equations has been doubled (possible only in multi-step mode).

NTRY a special option to simulate multiple entries. The user must set NTRY prior to using the calling sequence.

NTRY = 1 Setup entry (store all initial conditions first).

NTRY = 2 Normal Runge-Kutta/Cowell integration.

NTRY = 3 Integrate in Runge-Kutta mode exclusively.

(Note: NTRY = 1 must be used prior to the other two values. See Section II-B for further details.)

JHH an option to control the halving procedure.

JHH = 1 Reduce step size and return to Runge-Kutta mode.

JHH = 3 Return to previous step, restore all conditions (i. e., t , y_i , and y_i'') at that step, reduce step size and return to Runge-Kutta mode.

(Note: See Section II-C for exception to JHH = 3 option.)

JHD (No longer used in DEQ4)

All doubling is performed in the Cowell mode through the accumulation of alternate steps.

VMIN the location of one cell used by DEQ4 for the halving and doubling tests.

$VMIN = 10^{-1} ER/H^2$ (computed internally, varies with H)

Initially (prior to NTRY = 1) the user must set $VMIN \geq 1$, if TEST ≥ 2 (i. e., multi-step mode). This initial value allows the user to control the doubling procedure for the final N-IB equations if the multi-step mode is used. A larger value of VMIN (initially) will reduce the accuracy requirements for the final N-IB equations and thus allow them to be integrated at a larger step-size. A value of $10. \leq VMIN \leq 10.5$ is recommended.

VMAX the location of one cell used by DEQ4 for the halving and doubling tests. $VMAX = 10.3 ER/H^2$ (computed internally, varies with H).

T the location of the independent variable t_n -- stored initially by the user and incremented automatically by the subroutine during the integration procedure. T may be reset to a previous step by the subroutine during the starting procedure or, during the halving procedure when JHH = 3.

H the location of step-size h -- stored initially by the user and modified automatically by the subroutine during the integration procedure. Initially, DEQ4 sets $H = H/IR$ as the initial step-size for both Runge-Kutta and Cowell. If $H = 0$, DEQ4 sets $H = 0.01$ (H can be positive or negative). In the multi-step mode, H will contain the current step size of the first IB equations.

Y the location of N dependent variables y_i -- stored initially by the user and modified automatically by the subroutine during the integration procedure.

YP the location of N first derivatives y_i' -- stored initially by the user and modified automatically by the subroutine during the integration procedure.

Y2P the location of N second derivatives y_i'' -- computed and stored by the DAUX subroutine supplied by the user. If the two-group, multi-step mode is used, then DAUX should be programmed to skip the evaluation of the final N -IB second derivatives when TEST is negative.

T1 through are temporary storages used by the subroutine. Each T7, F2P, F1P, of these temporary storages must have a dimension and DLT1 of N and must be preserved throughout the integration through DLT8 procedure.

B. MULTIPLE ENTRIES

For purposes of compatibility between machines and different versions of Fortran IV, the parameter NTRY is used to simulate multiple entries. This requires the user to change the value of NTRY prior to using the calling sequence. This is done as follows:

NTRY = 1, Setup Entry

The user must set $NTRY = 1$ and store all initial conditions and options prior to using the calling sequence. This includes N , $I1$, $I2$, IB , IR , ER , $HMIN$, $HMAX$, $YMIN$, $TEST$, $NTRY$, JHH , $VMIN$, T , H , Y , and YP .

After setting $NTRY = 1$, the user must CALL DEQ4(N , $I1$, ..., $DLT8$) for the setup entry. The subroutine performs various tests on parameters (e. g. , sets $H = 0.01$, if $H = 0$), sets initial switches and options for the

integration procedure, calls DAUX to form y_1'' at t_0 , and then returns to the user. No integration is performed during the setup entry. The above entry must be performed prior to any other entry (one time only).

NTRY = 2, Integration Entry - Runge-Kutta/Cowell Mode

This is the normal integration entry and should be programmed within a DO loop (to control situations such as maximum steps in case of an error). After setting NTRY = 2, the user must CALL DEQ4(N, I1, ..., DLT8) to integrate one step in the Runge-Kutta/Cowell mode. The subroutine integrates one step (H/IR initially) and returns to the user. The first eight steps will be in the Runge-Kutta mode; thereafter the subroutine will integrate in the Cowell mode ($h = H/IR$), doubling approximately every 16 steps until $h \rightarrow H$. If the two-group, multi-step mode is used ($TEST \geq 2$ initially) then the step size of the final N-IB equations may continue to double, subject to the restrictions of the initial values of TEST and VMIN. In this case, during each entry to DEQ4, the first IB equations will be integrated R steps ($h = H$) while the final N-IB equations will be integrated one step ($h = R*H$). All of this is automatic, and the user need only loop through the calling sequence to integrate from t_0 to t_{END} . The user should test T after each integration step to determine the proper exit procedure, using NTRY = 3 to integrate to a specific time point t_{END} . If output is desired at a particular time point t_i ($t_i \neq t_n$), an interpolation subroutine such as RW NTRP is recommended.

NTRY = 3, Integrate in the Runge-Kutta Mode

After any integration step, or after setup entry, the user can integrate one or more steps in the Runge-Kutta mode. After setting NTRY = 3 (and changing the step-size H if necessary), the user must CALL DEQ4(N, I1, ..., DLT8) to integrate one step in the Runge-Kutta mode. The step size can be changed after each Runge-Kutta integration step, and negative H is permissible. NTRY = 3 should be used primarily to end the integration at a specific value t_{END} . It can also be used to integrate to a specific output

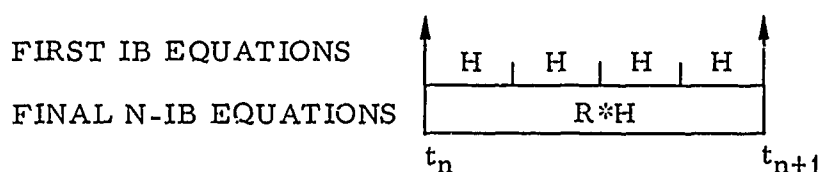
time t_{OUTPUT} ($t_n - H < t_{\text{OUTPUT}} < t_n + H$), where t_n is the current value of the independent variable and H is the current step size, if the regions TEST, T, H, Y, YF, Y2P, and T1 through T4 are saved and restored before continuing the normal integration (i. e., NTRY = 2). Note that the step size for the Runge-Kutta integration should be $\leq H/IR$ if the same accuracy is desired, where H is the current step size of the Cowell mode. If the two-group multi-step mode is used, then several Runge-Kutta steps may be required to integrate from t_n to t_{OUTPUT} (i. e., $t_n - R*H < t_{\text{OUTPUT}} < t_n + R*H$). (See Section II-C for further details.)

C. TWO-GROUP MULTI-STEP MODE

The subroutine assumes that the N equations can be separated into two groups (IB and N-IB) such that the first IB equations are not dependent on the final N-IB equations. This would be the case, for example, for a system of nonlinear differential equations which are integrated simultaneously with the variational equations (i. e., Newton-Raphson Method). Since the variational equations are always linear and also require less accuracy, they can be integrated at a larger step size than the first IB nonlinear differential equations. This is accomplished in DEQ4 through the use of the initial values of TEST and VMIN. TEST controls the maximum ratio of the two step sizes and VMIN controls the accuracy of the final N-IB equations. For example, if TEST = 3 and VMIN = 1000 initially, then the maximum possible ratio of the two groups will be $R_{\text{MAX}} = 2^2 = 2^{**}(\text{TEST} - 1)$ and the accuracy requirements for the final N-IB equations will be $\text{ER} * 1000$, where ER determines the accuracy of the first IB equations.

The doubling procedure works as follows: Initially, all N equations are integrated in the Runge-Kutta mode at a step-size $H = H_0/IR$. After eight Runge-Kutta steps all N equations are integrated in the Cowell mode at a step-size $h = H_0/IR$. Thereafter (assuming halving is not required), the step size for all N equations will double every 16 steps (in the Cowell mode) until the step size for the first IB equations can no longer be doubled. From

that point the step size of the final N-IB equations will continue to double under the restrictions of TEST and VMIN described above. For example, during an entry to DEQ4 (NTRY = 2) if R = 4 the following integration will be performed in the Cowell mode:



Note that during one entry into DEQ4, the first IB equations are integrated R steps with a step size of H while the final N -IB equations are integrated one step with a step size of $R*H$. Upon the next entry, if halving is required for the first IB equations, then H is reduced to $H = H/(2*IR)$ for all N equations and the above procedure is repeated. If $JHH = 1$ the integration will continue from $T = t_{n+1}$. If $JHH = 3$ the integration will normally continue from $T = t_n$ with all conditions restored at that point. However, if the final N -IB equations were being saved for doubling at $T = t_n$ (i.e., R_{MAX} had not been reached), then the integration will be continued from $T = t_{n+1}$ (same as $JHH = 1$). Thus, the doubling of the final N -IB equations is given precedent over the halving procedure in regards to the $JHH = 3$ option. For this reason $TEST \leq 5$ is recommended, since the doubling procedure for the final N -IB equations is discontinued when R_{MAX} has been reached.

Since 2(R-1)(N-IB) derivatives are no longer computed during each Cowell step, the use of the two-group multi-step mode will result in a considerable saving of computing time where applicable.

D. CODING INFORMATION

The calling sequence can be simplified to

CALL DEQ4

by placing all parameters of the calling sequence in (labeled or blank)
COMMON and using the name DAUX (identical with the name used internally

by DEQ4) for the auxiliary subroutine. In addition, all parameters (i. e. , Y, YP, Y2P, etc.) must be dimensioned within subroutine DEQ4¹, and the SUBROUTINE statement in DEQ4 must be changed to

SUBROUTINE DEQ4

E. SPACE REQUIRED

In addition to the parameters in the calling sequence, approximately 3571₈ cells are required.

Note: The coefficients required for the Cowell integration mode are stored in DEQ4 as 20 digital octal constants through the use of the DATA declaration. These coefficients were formed in double precision on the CDC 6600 and are the octal equivalent of the 60-bit real floating point constants of the CDC 6000 series machines. See Appendix A for a complete description of the mathematical method.

¹ The Fortran IV Source Language for DEQ4 is provided in Appendix B.

APPENDIX A

MATHEMATICAL METHOD

The ASC DEQ4 subroutine [Floating Point Cowell (Second-Sum) Runge-Kutta Integration of Second-Order Ordinary Differential Equations] is prepared to solve the system of equations defined as

$$\begin{aligned} y_i'' &= f_i(t, y_1, \dots, y_N, y_1', \dots, y_N') \quad (i = 1, 2, \dots, N) \\ y_i(t_0) &= y_{i0}, \quad y_i'(t_0) = y_{i0}' \quad (i = 1, 2, \dots, N) \end{aligned} \tag{A-1}$$

In case none of the f_i involve the first derivatives y_i' , time is saved by indicating this in the set-up (i.e., set I1 = -1). DEQ4 includes a fourth order Runge-Kutta subroutine that is used for the starting procedure and for the halving procedure. The Runge-Kutta subroutine can also be used independently of the main subroutine through the use of NTRY = 3. For the sake of completeness the Runge-Kutta equations are given in the following paragraphs.

A. 1. RUNGE-KUTTA EQUATIONS

Let y_{in} and y_{in}' be the values of y_i and y_i' at $t = t_n$; f_{in} be the second derivative of y_i at $t = t_n$; and h be the increment (step size) of the independent variable t . The Runge-Kutta formulas¹ used in this subroutine are as follows:

¹J. B. Scarborough, Numerical Mathematical Analysis, Third Edition, John Hopkins Press, Baltimore, Maryland (1955) pp. 300-301.

$$k_{i1} = hf_i(t_n, y_{in}, y'_{in})$$

$$k_{i2} = hf_i\left(t_n + \frac{h}{2}, y_{in} + \frac{h}{2}y'_{in} + \frac{h}{8}k_{i1}, y'_{in} + \frac{k_{i1}}{2}\right)$$

$$k_{i3} = hf_i\left(t_n + \frac{h}{2}, y_{in} + \frac{h}{2}y'_{in} + \frac{h}{8}k_{i1}, y'_{in} + \frac{k_{i2}}{2}\right)$$

$$k_{i4} = hf_i(t_n + h, y_{in} + hy'_{in} + \frac{h}{2}k_{i3}, y'_{in} + k_{i3}) \quad (A-2)$$

$$\Delta y_{in} = h\left[y'_{in} + \frac{1}{6}(k_{i1} + k_{i2} + k_{i3})\right]$$

$$\Delta y'_{in} = \frac{1}{6}[k_{i1} + 2k_{i2} + 2k_{i3} + k_{i4}]$$

$$y_{i, n+1} = y_{in} + \Delta y_{in}$$

$$y'_{i, n+1} = y'_{in} + \Delta y'_{in}$$

For the special second-order equation, you have

$$y''_i = f_i(t, y_1, \dots, y_n) \quad (1st \text{ derivatives missing}) \quad (A-3)$$

It should be noted that $k_{i2} = k_{i3}$, so that above formulas reduce to the following Runge-Kutta formulas:

$$k_{i1} = hf_i(t_n, y_{in})$$

$$k_{i2} = hf_i\left(t_n + \frac{h}{2}, y_{in} + \frac{h}{2}y'_{in} + \frac{h}{8}k_{i1}\right)$$

$$k_{i3} = hf_i\left(t_n + h, y_{in} + hy'_{in} + \frac{h}{2}k_{i2}\right)$$

$$\Delta y_{in} = h\left[y'_{in} + \frac{1}{6}(k_{i1} + 2k_{i2})\right]$$

(cont.)

$$\Delta y'_{in} = \frac{1}{6} [k_{i1} + 4k_{i2} + k_{i3}]$$

$$y_{i, n+1} = y_{in} + \Delta y_{in}$$

$$y'_{i, n+1} = y'_{in} + \Delta y'_{in} \quad (A-4)$$

where k_{i4} of Eq. (A-2) is now k_{i3} of Eq. (A-4).

The subroutine can be made to take advantage of this fact by a simple change in the calling sequence (i. e. , set I1 = -1) and thus save one derivative per integration step in the Runge-Kutta mode.

A. 2 COWELL STARTING PROCEDURE

A Cowell (Second-Sum) method based on eight differences is used to continue the integration after the first eight Runge-Kutta steps. The user must ask for each integration step and the subroutine will follow this sequence:

- a. Perform eight Runge-Kutta steps of size $h = H_{start}/IR$ (one Runge-Kutta step for each entry to DEQ4) to obtain $y_{i1}, y'_{i1}, y''_{i1}$ through $y_{i8}, y'_{i8}, y''_{i8}$.
- b. For each of the N equations, that part of the difference table above the diagonal line is constructed in an accumulative manner during the eight Runge-Kutta steps (DEQ4 returns to the user after each Runge-Kutta step).

To start the Cowell integration we need $''F_{i10}, 'F_{i9}, y_{i8}, y'_{i8}, y''_{i8}, \Delta_{i7}^I, \Delta_{i6}^{II}, \Delta_{i5}^{III}, \Delta_{i4}^{IV}, \Delta_{i3}^V, \Delta_{i2}^{VI}, \Delta_{i1}^{VII}$, and Δ_{i0}^{VIII} . The values y_{i8}, y'_{i8} , and y''_{i8} are available after the eight Runge-Kutta integration step. The other values are computed as follows:

$$\begin{aligned} 'F_{i9} = & y'_{i4}/H + W_0 y''_{i0} + W_1 y''_{i1} + W_2 y''_{i2} + W_3 y''_{i3} \\ & + W_4 y''_{i4} + W_5 y''_{i5} + W_6 y''_{i6} + W_7 y''_{i7} + W_8 y''_{i8} \end{aligned} \quad (A-5)$$

$$\begin{aligned} {}''F_{i10} = & y_{i4}/H^2 + 5y'_{i4}/H + V_0 y''_{i0} + V_1 y''_{i1} + V_2 y''_{i2} \\ & + V_3 y''_{i3} + V_4 y''_{i4} + V_5 y''_{i5} + V_6 y''_{i6} + V_7 y''_{i7} + V_8 y''_{i8} \end{aligned} \quad (A-6)$$

$$\Delta_{i7}^I = y''_{i8} - y''_{i7} \quad (A-7)$$

$$\Delta_{i6}^{II} = y''_{i8} - 2y''_{i7} + y''_{i6} \quad (A-8)$$

$$\Delta_{i5}^{III} = y''_{i8} - 3y''_{i7} + 3y''_{i6} - y''_{i5} \quad (A-9)$$

$$\Delta_{i4}^{IV} = y''_{i8} - 4y''_{i7} + 6y''_{i6} - 4y''_{i5} + y''_{i4} \quad (A-10)$$

$$\Delta_{i3}^V = y''_{i8} - 5y''_{i7} + 10y''_{i6} - 10y''_{i5} + 5y''_{i4} - y''_{i3} \quad (A-11)$$

$$\Delta_{i2}^{VI} = y''_{i8} - 6y''_{i7} + 15y''_{i6} - 20y''_{i5} + 15y''_{i4} - 6y''_{i3} + y''_{i2} \quad (A-12)$$

$$\Delta_{i1}^{VII} = y''_{i8} - 7y''_{i7} + 21y''_{i6} - 35y''_{i5} + 35y''_{i4} - 21y''_{i3} + 7y''_{i2} - y''_{i1} \quad (A-13)$$

$$\begin{aligned} \Delta_{i0}^{VIII} = & y''_{i8} - 8y''_{i7} + 28y''_{i6} - 56y''_{i5} \\ & + 70y''_{i4} - 56y''_{i3} + 28y''_{i2} - 8y''_{i1} + y''_{i0} \end{aligned} \quad (A-14)$$

Before going to a Cowell step, the step-size $h = H_{\text{start}}/IR$ is tested. Only the first IB equations are used to test, where $1 \leq IB \leq N$. For the first

IB equations we determine

$$V = \frac{\max_{1 \leq i \leq IB}}{\left[\frac{|\Delta_{i1}^{VII}|}{\max(|y_{i8}|, YMIN)} \right]} \quad (A-15)$$

If $V \geq 10^3 * ER/h^2$, then the ratio of the seventh difference to function is too large. Therefore, h is reduced to $h = h/(2 * IR)$, the initial conditions (i. e., t_0 , y_{i0} , y'_{i0} , and y''_{i0}) are restored, and the integration procedure is restarted. This procedure is repeated until: (a) $V < 10^3 * ER/h^2$ or (b) $h < HMIN$. For (a) the routine proceeds to a Cowell integration step with the current value of h . For (b) the routine sets $TEST = 13$ and returns to the user -- indicating a programming error or that ER , H_{start} , or $HMIN$ are too restrictive. The constant $YMIN$ (equals 1. if unspecified) prevents division by y near a zero; for example, in the sine calculation $YMIN = 0.01$ avoids difficulty near 180 deg. The value ER (equals $1E - 11$ if unspecified) allows a larger h if chosen larger, say $ER = 1E - 8$.

A.3 COWELL INTEGRATION

If $V < 10^3 * ER/h^2$ after the eighth Runge-Kutta step, we begin the Cowell integration with predictions of

$$y_{i9} = h^2 \left(F_{i10} + N_0 y''_{i8} + N_1 \Delta_{i7}^I + N_2 \Delta_{i6}^{II} + N_3 \Delta_{i5}^{III} + N_4 \Delta_{i4}^{IV} + N_5 \Delta_{i3}^V + N_6 \Delta_{i2}^{VI} + N_7 \Delta_{i1}^{VII} + N_8 \Delta_{i0}^{VIII} \right) \quad (A-16)$$

$$y'_{i9} = h \left(F_{i9} + N_0 y'_{i8} + N_1 \Delta_{i7}^I + N_2 \Delta_{i6}^{II} + N_3 \Delta_{i5}^{III} + N_4 \Delta_{i4}^{IV} + N_5 \Delta_{i3}^V + N_6 \Delta_{i2}^{VI} + N_7 \Delta_{i1}^{VII} + N_8 \Delta_{i0}^{VIII} \right) \quad (A-17)$$

These equations use the row of the difference table above the diagonal line; only this row is needed for a Cowell step and is kept up to date as the integration proceeds. The prediction for y'_{i9} is omitted if the option I1 = -1 is used. Now from y_{i9} and y'_{i9} , we obtain y''_{i9} (from DAUX) and then complete the row of differences out to Δ_{i1}^{VIII} under the diagonal line in Table A-1. For example: $\Delta_{i8}^I = y''_{i9} - y'_{i8}$; $\Delta_{i7}^{II} = \Delta_{i8}^I - \Delta_{i7}^I$; and so on.

With this row, we calculate the corrected values:

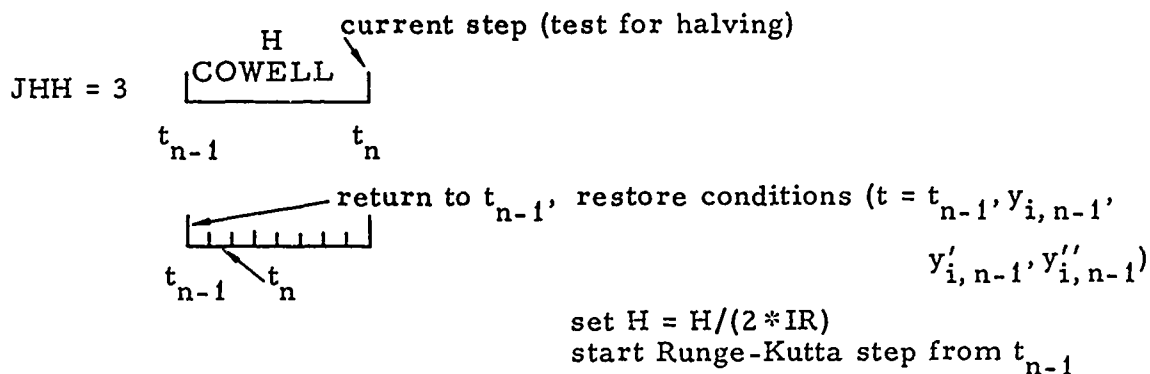
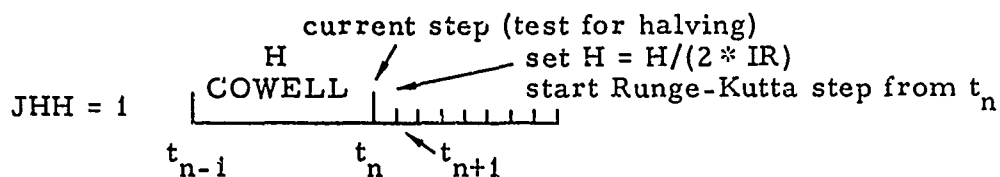
$$y_{i9} = h^2 \left('F_{i10} + B_0 y''_{i9} + B_1 \Delta_{i8}^I + B_2 \Delta_{i7}^{II} + B_3 \Delta_{i6}^{III} + B_4 \Delta_{i5}^{IV} + B_5 \Delta_{i4}^V + B_6 \Delta_{i3}^{VI} + B_7 \Delta_{i2}^{VII} + B_8 \Delta_{i1}^{VIII} \right) \quad (A-18)$$

$$y'_{i9} = h \left('F_{i9} + \dot{B}_0 y''_{i9} + \dot{B}_1 \Delta_{i8}^I + \dot{B}_2 \Delta_{i7}^{II} + \dot{B}_3 \Delta_{i6}^{III} + \dot{B}_4 \Delta_{i5}^{IV} + \dot{B}_5 \Delta_{i4}^V + \dot{B}_6 \Delta_{i3}^{VI} + \dot{B}_7 \Delta_{i2}^{VII} + \dot{B}_8 \Delta_{i1}^{VIII} \right) \quad (A-19)$$

From these we get corrected values for y''_{i9} (from DAUX) and recalculate the entire row under the diagonal line. Using these new values we calculate new values for y_{i9} and y'_{i9} using Eqs. (A-18) and (A-19). Thus, y_{i9} and y'_{i9} are corrected twice; however, new values for y''_{i9} are not computed for these new values. Next we compute $'F_{i10} = 'F_{i9} + y''_{i9}$ and $''F_{i11} = ''F_{i10} + 'F_{i10}$. This completes the integration step and DEQ4 exits to the user.

On the next entry we repeat the test for halving [i. e., at Eq. (A-15)]. If halving is not required, we continue the Cowell integration using Eqs. (A-16) through (A-19) as before. If halving is required after at least one Cowell integration step has been completed, we set $H = H/(2 * IR)$ and start a new sequence of eight Runge-Kutta steps. If JHH = 1, we do not retrace ground; however, if JHH = 3 (and the final N-IB equations are not being saved for doubling in the two-group multi-step mode) then we return to the previous step, restore the conditions at that point and then start a new sequence of

eight Runge-Kutta steps with $H = H/(2 * IR)$. This can be shown graphically as



During the halving procedure all N equations return to Runge-Kutta with the same step size (i. e. , the two-group multi-step mode is temporarily suspended).

If halving is not required, we proceed with a Cowell step, making the following test every other step to determine whether we may be able to double h . If

$$V \leq \frac{(10^{-2}) * ER}{h^2} \quad (A-20)$$

we may be able to double h .

We test further to see that

$$W = \frac{\max_{1 \leq i \leq IB}}{\left[\frac{|\Delta_{10}^{VIII}|}{\max(|y_{i8}|, YMIN)} \right]} \leq \frac{10^{-2} * ER}{h^2} \quad (A-21)$$

If the conditions of Eqs. (A-20) and (A-21) are satisfied for 16 steps (testing every other step) then the step-size h is doubled for all N equations in the Cowell mode. In addition, all of the data above the diagonal line is doubled in the Cowell mode using Eq. (A-23). We then proceed to a Cowell step using Eqs. (A-16) through (A-19) with step-size $2H$. On the next entry, the halving and doubling tests are continued as before.

The doubling procedure requires a counting device and it works as follows. Initially, we set $K = 1$ at the beginning of the first Cowell step. The counter is advanced every other step if Eqs. (A-20) and A-21 are satisfied for the first IB equations. We accumulate the data required for doubling at alternate steps. If the tests fail at any point (assuming halving is not required) the counter is restarted if all N equations are being integrated at the same step size (i. e. , $TEST = VMIN = 1$. initially). However, if the two-group mode is being used, then the doubling tests for the first IB equations are temporarily suspended (i. e. , the step size for the first IB equations remains constant unless halving is later required). Thereafter, the doubling for the final N -IB equations is continued using the following test, that is, if

$$VAR = \frac{\max_{IB < i \leq N}}{\left[\frac{|\Delta_{i1}^{VII}|}{\max(|y_{i8}|, YMIN)} \right]} < \frac{10^{-2} * ER * VMIN}{h^2} \quad (A-22)$$

for the remaining steps [$K = 1(1)9$], then the step size for the final N -IB equations is doubled. Also, for the final N -IB equations all of the data above the diagonal line is doubled in the Cowell mode. Note that $VMIN$ of Eq. (A-22) is the initial value of $VMIN$ for $NTRY = 1$. The counter K will be set to one for the next entry, and the doubling procedure will be restarted for the final N -IB equations.

The equations used for doubling in the Cowell mode are as follows. Let Δ represent a difference (i. e. , $\Delta^I = \Delta_{17}^I$, $\Delta^{II} = \Delta_{16}^{II}$) at step-size h, and \blacktriangle represent a difference at step-size 2h. Then we compute

$$\begin{aligned}
 \blacktriangle^I &= 2\Delta^I - \Delta^{II} \\
 \blacktriangle^{II} &= 4\Delta^{II} - (4\Delta^{III} - \Delta^{IV}) \\
 \blacktriangle^{III} &= 8\Delta^{III} - (12\Delta^{IV} - 6\Delta^V + \Delta^{VI}) \\
 \blacktriangle^{IV} &= 16\Delta^{IV} - (32\Delta^V - 24\Delta^{VI} + 8\Delta^{VII} - \Delta^{VIII}) \\
 \blacktriangle^V &= 5\blacktriangle^{IV} - (10\blacktriangle^{III} - 10\blacktriangle^{II} + 5\blacktriangle^I) + (y_{16}'' - y_6'') \\
 \blacktriangle^{VI} &= 6\blacktriangle^V - (15\blacktriangle^{IV} - 20\blacktriangle^{III} + 15\blacktriangle^{II} - 6\blacktriangle^I) - (y_{16}'' - y_4'') \\
 \blacktriangle^{VII} &= 7\blacktriangle^{VI} - (21\blacktriangle^V - 35\blacktriangle^{IV} + 35\blacktriangle^{III} - 21\blacktriangle^{II} + 7\blacktriangle^I) + (y_{16}'' - y_2'') \\
 \blacktriangle^{VIII} &= 8\blacktriangle^{VII} - (28\blacktriangle^{VI} - 56\blacktriangle^V + 70\blacktriangle^{IV} - 56\blacktriangle^{III} + 28\blacktriangle^{II} - 8\blacktriangle^I) - (y_{16}'' - y_0'') \\
 'F(\blacktriangle) &= y_8'/2h + W_0 y_0'' + W_1 y_2'' + W_2 y_4'' + W_3 y_6'' \\
 &\quad + W_4 y_8'' + W_5 y_{10}'' + W_6 y_{12}'' + W_7 y_{14}'' + W_8 y_{16}'' \\
 ''F(\blacktriangle) &= y_8/(2h)^2 + 5 y_8'/2h + V_0 y_0'' + V_1 y_2'' + V_2 y_4'' \\
 &\quad + V_3 y_6'' + V_4 y_8'' + V_5 y_{10}'' + V_6 y_{12}'' + V_7 y_{14}'' + V_8 y_{16}'' \quad (A-23)
 \end{aligned}$$

where the values y_8 , y_8' , and y_0'' , y_2'' , ..., y_{16}'' are the integrated values saved at alternate steps of the Cowell integration procedure. For the two-group mode h will be the value in cell H when the step size for all N equations is being doubled and R * H when the step size for the final N-IB equations is being doubled.

A. 4 CALCULATION OF COEFFICIENTS

In a previous version of the subroutine (ASC DEQ2) $''F_{i10}$ and $'F_{i9}$ of Table A-1 were calculated by first forming $''F_{i5}$ and $'F_{i5}$ as follows:

$$\begin{aligned} 'F_{i5} = & y'_{i4}/H - D_0 y''_{i4} - D_1 \Delta_{i4}^I - D_2 \Delta_{i3}^{II} - D_3 \Delta_{i3}^{III} \\ & - D_4 \Delta_{i2}^{IV} - D_5 \Delta_{i2}^V - D_6 \Delta_{i1}^{VI} - D_7 \Delta_{i1}^{VII} - D_8 \Delta_{i0}^{VIII} \end{aligned} \quad (A-24)$$

$$''F_{i5} = y_{i4}/H^2 - C_0 y''_{i4} - C_2 \Delta_{i3}^{II} - C_4 \Delta_{i2}^{IV} - C_6 \Delta_{i1}^{VI} - C_8 \Delta_{i0}^{VIII} \quad (A-25)$$

Then $''F_{i10}$ and $'F_{i9}$ are calculated through the sequence as

$$'F_{iK+1} = 'F_{iK} + y''_{iK} \quad (K = 5, 6, \dots, 8) \quad (A-26)$$

$$''F_{iK+1} = ''F_{iK} + 'F_{iK} \quad (K = 5, 6, \dots, 9) \quad (A-27)$$

However, by substituting ordinates (y''_{iK}) for differences (Δ_{iK}) (e. g., $\Delta_{i4}^I = y''_{i5} - y''_{i4}$; $\Delta_{i3}^{II} = y''_{i5} - 2y''_{i4} + y''_{i3}$) in Eqs. (A-24) and (A-25) and through the use of Eqs. (A-26) and (A-27) $'F_{i9}$ and $''F_{i10}$ can be defined by Eqs. (A-5) and (A-6). Tables A-2 and A-3 give the value of V_i and W_i . Table A-4 gives the values of the other coefficients.

The coefficients for V_i and W_i were formed in double precision on the CDC 6600 and are included in subroutine DEQ4 as 20 digit octal constants. For example, using Table A-3

$$V_7 = (2 - 5D5 - 5D6 + 35D7 + 40D8 - C6 + 8C8) \quad (A-28)$$

Table A-2. Coefficients for W_i for Eq. (A-5)

	1	D_0	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8
W_0										-1
W_1								-1	1	8
W_2						-1	1	6	-7	-28
W_3				-1	1	4	-5	-15	21	56
W_4		-1	1	2	-3	-6	10	20	-35	-70
W_5	1		-1	-1	3	4	-10	-15	35	56
W_6	1				-1	-1	5	6	-21	-28
W_7	1						-1	-1	7	8
W_8	1								-1	-1

Table A-3. Coefficients for V_i for Eq. (A-6)

	1	D_0	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	C_0	C_2	C_4	C_6	C_8
V_0										-5					-1
V_1								-5	5	40				-1	8
V_2						-5	5	30	-35	-140			-1	6	-28
V_3				-5	5	20	-25	-75	105	280		-1	4	-15	56
V_4		-5	5	10	-15	-30	50	100	-175	-350	-1	2	-6	20	-70
V_5	4		-5	-5	15	20	-50	-75	175	280		-1	4	-15	56
V_6	3				-5	-5	25	30	-105	-140			-1	6	-28
V_7	2						-5	-5	35	40				-1	8
V_8	1								-5	-5					-1

Table A-4. Coefficients for N_i , \dot{N}_i , B_i , \dot{B}_i , D_i , and C_i

$i =$	0	1	2	3	4	5	6	7	8
N_i	$\frac{1}{12}$	$\frac{1}{12}$	$\frac{19}{240}$	$\frac{3}{40}$	$\frac{863}{12096}$	$\frac{275}{4032}$	$\frac{33953}{518400}$	$\frac{8183}{129600}$	$\frac{3250433}{53222400}$
\dot{N}_i	$\frac{1}{2}$	$\frac{5}{12}$	$\frac{3}{8}$	$\frac{251}{720}$	$\frac{95}{288}$	$\frac{19087}{50480}$	$\frac{5257}{17280}$	$\frac{1070017}{3628800}$	$\frac{25713}{89600}$
B_i	$\frac{1}{12}$	0	$-\frac{1}{240}$	$-\frac{1}{240}$	$-\frac{221}{60480}$	$-\frac{19}{6048}$	$-\frac{9829}{3628800}$	$-\frac{407}{172800}$	$-\frac{330157}{159667200}$
\dot{B}_i	$\frac{1}{2}$	$-\frac{1}{12}$	$-\frac{1}{24}$	$-\frac{19}{720}$	$-\frac{3}{160}$	$-\frac{863}{60480}$	$-\frac{275}{24192}$	$-\frac{33953}{3628800}$	$-\frac{8183}{1036800}$
D_i	$-\frac{1}{2}$	$-\frac{1}{12}$	$\frac{1}{24}$	$\frac{11}{720}$	$-\frac{11}{1440}$	$-\frac{191}{60480}$	$\frac{191}{120960}$	$\frac{2497}{3628800}$	$-\frac{2497}{7257600}$
C_i	$\frac{1}{12}$	0	$-\frac{1}{240}$	0	$\frac{31}{60480}$	0	$-\frac{289}{3628800}$	0	$\frac{317}{22809600}$

APPENDIX B

FORTRAN IV SOURCE LANGUAGE FOR DEQ4
(CDC 6400-6600)

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C   ASC DEQ4 (8TH ORDER) R.K./GAUSS JACKSON (4-18-67) J.F. HOLT      DEQ40001
      SUBROUTINE DEQ4(N,I1,I2,IA,IB,IR,ER,HMIN,HMAX,YMIN,DAUX,TEST,IDH, DEQ40002
1     NTRY,JHH,JHD,VMIN,VMAX,      DEQ40003
2     T,H,Y,YP,Y2P,T1,T2,T3,T4,   DEQ40004
3     T5,T6,T7,                     DEQ40005
4     F2P,F1P,DLT1,DLT2,DLT3,DLT4,DLT5,DLT6,DLT7,DLT8)             DEQ40006
      DATA A0,A1,A2,A3,A4,A5,A6,A7,A8/017145252525252525252,017145252525252525252,017145042104210421042,017144631463146314631,01714444167144441671,0171442727272727272,017144142124345450046,0171440247700247700,017137642352047260270/
      DATA AP0,AP1,AP2,AP3,AP4,AP5,AP6,AP7,AP8/01717400000000000000,017166525252525252525,01716600000000000000,017165447644764476447,017165216161616161616,017165031250377565231,017164674152142466774,017164557436021207661,017164456716206452330/
      DATA B0,B1,B2,B3,B4,B5,B6,B7,B8/017145252525252525252,00000000000000000000,0060673567356735673567,006070041031300410313,0060701441671441671441,0060702347642525026560,0060703132207031322,0060703607613672523307/
      DATA BP0,BP1,BP2,BP3,BP4,BP5,BP6,BP7,BP8/01717400000000000000,00606325252525252525,00606425252525252525,006065117511751175,0060653146314631463,0060660543327060160543,0060662134066134066134,0060663153172725033257,0060663753007252122331/
      DATA W0,W1,W2,W3,W4,W5,W6,W7,W8/017045506100743107612,0060700423525004235,00607124634350133463213,0060633425400145555331,00607174000000000000,00607204216517771511122,00607177663070575106313,0060720400735400735,00607224266406711557615,00607215636363515616135,006072140226620071160620,0060717770713144246212/
C   THE CALLING SEQUENCE CAN BE SIMPLIFIED BY PUTTING ALL PARAMETERS DEQ40030
C   EXCEPT NTRY AND DAUX IN LABELED COMMON. (SEE EXAMPLE BELOW)      DEQ40031
C   HOWEVER, THE DIMENSION STATEMENTS MUST BE CHANGED, OR INCLUDED    DEQ40032
C   IN THE LABELLED COMMON STATEMENT. THE NEW CALLING SEQ. BECOMES    DEQ40033
C   CALL DEQ4 (NTRY,DAUX)                                               DEQ40034
C   ALSO, THE SUBROUTINE STATEMENT (SEE ABOVE) MUST BE CHANGED TO     DEQ40035
C   SUBROUTINE DEQ4(NTRY,DAUX)                                          DEQ40036
C   EXAMPLE FOLLOWING SHOWS LABELED COMMON FOR SIMPLIFIED CALLING SEQ. DEQ40037
C   COMMON/CDEQ/N,I1,I2,IA,IB,IR,ER,HMIN,HMAX,YMIN,TEST,IDH,IRK,JHH, DEQ40038
C   1     JHD,VMIN,VMAX,T,H,Y,YP,Y2P,T1,T2,T3,T4,T5,T6,T7,           DEQ40039
C   2     F2P,F1P,DLT1,DLT2,DLT3,                                     DEQ40040
C   3     DLT4,DLT5,DLT6,DLT7,DLT8                                    DEQ40041

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C      DIMENSION Y( 63),YP( 63),Y2P( 63),T1( 63),T2( 63),T3( 63),      DEQ40043
C      1      T4( 63),T5( 63),T6( 63),T7( 63),      DEQ40044
C      2      F2P( 63),F1P( 63),DLT1( 63),DLT2( 63),      DEQ40045
C      3      DLT3( 63),DLT4( 63),DLT5( 63),DLT6( 63),DLT7( 63),      DEQ40046
C      4      DLT8( 63)      DEQ40047
      DIMENSION Y(2),YP(2),Y2P(2),T1(2),T2(2),T3(2),T4(2)      DEQ40048
      DIMENSION T5(2),T6(2),T7(2)      DEQ40049
      DIMENSION F2P(2),F1P(2)      DEQ40050
      DIMENSION DLT1(2),DLT2(2),DLT3(2),DLT4(2),DLT5(2),DLT6(2)      DEQ40051
      DIMENSION DLT7(2),DLT8(2)      DEQ40052
C*****NOTE ALL OPTIONS AND INITIAL CONDITIONS (T,H,Y,YP) MUST BE STORED DEQ40053
C***** PRIOR TO THE SETUP ENTRY TO DEQ4. (DEQ4 ENTRY CALLS DAUX) DEQ40054
C***** SPECIAL NOTE ***** SPECIAL NOTE *****CDEQ40055
C      WITH THE DATA ALLOCATION SCHEME OF DEQ4, IT IS POSSIBLE FOR DEQ40056
C      THE USER TO INTEGRATE THE FIRST P EQUATIONS SIMPLY BY CHANGING N. DEQ40057
C      OF COURSE, THIS ASSUMES THAT THE FIRST P EQUATIONS DO NOT DEPEND DEQ40058
C      ON THE FINAL N-P EQUATIONS. (SEE WRITE-UP FOR FURTHER DETAILS.) DEQ40059
C      N      IS THE NUMBER OF EQUATIONS. DEQ40060
C      I1      IS AN OPTION, SUCH THAT IF DEQ40061
C      I1 IS G.E. +n, Y2P = F(X,Y,YP) (I.E., FUNCTION OF 1ST DERIV.) DEQ40062
C      I1 IS L.T. 0, Y2P = F(X,Y) DEQ40063
C      I2      IS AN OPTION, SUCH THAT IF DEQ40064
C      I2 IS G.E. +n, VARIABLE STEP-SIZE MODE IS USED. DEQ40065
C      I2 IS L.T. 0, FIXED STEP-SIZE MODE IS USED. DEQ40066
C      IA      IS AN INDICATOR SWITCH TO THE USER DURING EXIT TO DAUX SUB. DEQ40067
C      IA=-1 FOR 1ST (1,2,3 IF R.K.) PASS THRU DAUX. DEQ40068
C      IA=+1 FOR FINAL PASS THRU DAUX. (APPLIES FOR EACH STEP.) DEQ40069
C      NOTE    IN THE COWELL MODE, IA=-1 WHEN THE DERIVATIVES OF THE DEQ40070
C      PREDICTOR ARE BEING ASKED FOR, AND IA=+1 WHEN THE DEQ40071
C      DERIVATIVES OF THE CORRECTOR ARE BEING ASKED FOR. DEQ40072
C      IB      ONLY THE 1ST IB (I.E. N) EQNS. ARE TESTED DURING ERROR TESTS. DEQ40073
C      FOR THE TWO GROUP MODE, THE FIRST IB EQNS ARE INTEGRATED AT DEQ40074
C      STEP-SIZE H, AND THE FINAL N-IB EQNS ARE INTEGRATED AT STEP- DEQ40075
C      SIZE R*H (R= 1., 2., 4., 8., ETC. DEPENDING ON THE INITIAL DEQ40076
C      VALUES OF TEST AND VMIN). (SEE TEST AND VMIN) DEQ40077
C      IR      FOR A GIVEN STEP-SIZE H, COWELL STEP = H, R.K. STEP = H/IR. DEQ40078
C      ER      RELATIVE ERROR CRITERIA. (SET ER=1.E-9 OR LESS) DEQ40079
C      HMIN     IS THE MINIMUM STEP-SIZE ALLOWED. (ABSOLUTE VALUE) DEQ40080
C      HMAX     IS THE MAXIMUM STEP-SIZE ALLOWED. (ABSOLUTE VALUE) DEQ40081
C      YMIN     IS THE MIN. ABS. VALUE OF Y(I) ALLOWED FOR THE ERROR TEST. DEQ40082
C      DAUX     IS AN EXTERNAL SUB. SUPPLIED BY USER TO EVAL. THE 2ND DERIV. DEQ40083
C      TEST     AFTER EACH INTEGRATION STEP, DEQ40084

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C      TEST WILL BE +1. IF THE INTEGRATION WAS A RUNGE-KUTTA STEP. DEQ40085
C      TEST WILL BE -1. IF THE INTEGRATION WAS A COWELL STEP. DEQ40086
C      NOTE INITIALLY SET TEST=1. FOR NORMAL INTEGRATION. FOR TWO-DEQ40087
C      GROUP MODE SET TEST G.E. 2. (MAX R = 2.** (TEST-1.) DEQ40088
C      IDH AFTER EACH INTEGRATION STEP. DEQ40089
C      IDH WILL BE +1 IF THE STEP-SIZE HAS NOT CHANGED. DEQ40090
C      IDH WILL BE +2 IF THE STEP-SIZE HAS BEEN HALVED. DEQ40091
C      IDH WILL BE +3 IF THE STEP-SIZE HAS BEEN DOUBLED DEQ40092
C      IDH WILL BE +4 IF H FOR FINAL N-IB EQNS. DOUBLED. DEQ40093
C      NTRY IS A SPECIAL OPTION TO ALLOW MULTIPLE ENTRIES. DEQ40094
C      NTRY=1, SETUP ENTRY. (STORE INITIAL COND. PRIOR TO ENTRY.) DEQ40095
C      NTRY=2, NORMAL R.K./GAUSS-JACKSON INTEGRATION. DEQ40096
C      NTRY=3, INTEGRATE IN R.K. MODE EXCLUSIVELY. DEQ40097
C      JHH IS AN OPTION TO CONTROL THE HALVING PROCEDURE. IF, DEQ40098
C      JHH=1, 8*IR R.K. STEPS ARE USED DURING THE HALVING PROCEDURE. DEQ40099
C      JHH=3, RETURN TO T(I) AFTER COWELL ATTEMPT TO T(I+1), 8*IR RK DEQ40100
C      SEE WRITE-UP FOR FURTHER DETAILS CONCERNING HALVING PROCEDURE DEQ40101
C      JHD IS AN OPTION TO CONTROL THE DOUBLING PROCEDURE. DEQ40102
C      NOTE JHD IS NO LONGER USED IN DEQ4. ALL DOUBLING IS DONE DEQ40103
C      IN THE COWELL MODE BY THE ACCUM. OF ALTERNATE DATA. DEQ40104
C      VMIN IS THE LOC OF 1 CELL USED BY DDEQ FOR HALVING/DOUBLING TEST DEQ40105
C      NOTE INITIALLY SET VMIN=1, EP (P=2,3,...,5) FOR TWO-GROUP MODE DEQ40106
C      VMAX IS THE LOC OF 1 CELL USED BY DDEQ FOR HALVING/DOUBLING TEST DEQ40107
C      T IS THE LOCATION OF THE INDEPENDENT VARIABLE T(I). DEQ40108
C      H IS THE LOCATION OF THE INITIAL AND CURRENT STEP-SIZE. DEQ40109
C      Y IS THE LOCATION OF N DEPENDENT VARIABLES. DEQ40110
C      YP IS THE LOCATION OF N 1ST DERIVATIVES. DEQ40111
C      Y2P IS THE LOCATION OF N 2ND DERIVATIVES. (COMPUTED BY DAUX) DEQ40112
C      T1 THRU T7 ARE VECTORS OF DIMENSION N USED BY THE SUBROUTINE. DEQ40113
C      F2P, F1P, AND DLT1 THRU DLT8 ARE VECTORS OF DIMENSION N. DEQ40114
C      SETUP FOR DEQ4 SUBROUTINE. CALL DEQ4(N,I1,I2,...,DLT7,DLT8) DEQ40115
C      GO TO (1,2,3),NTRY DEQ40116
1      IDH=1 DEQ40117
      RXH=TEST DEQ40118
      IF (RXH=1,) 380,381,381 DEQ40119
380  RXH=1. DEQ40120
381  IKR=1 DEQ40121
      IF (VMIN=1,) 382,383,383 DEQ40122
382  VMIN=1000. DEQ40123
383  VARX=VMIN DEQ40124
      RXA=RXH DEQ40125
      TEST=+1. DEQ40126

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TST=+1,
NSTR1=-1
IF (N) 391,390,392
390 N=1
391 N=IABS(N)
392 IF (N-IR) 393,394,394
393 IR=N
394 IF (IR) 400,400,410
400 IR=N
410 IF (IR) 420,420,430
420 IR=16
430 IF (H) 432,431,432
431 H=.01
C431 H=.01D0
432 R=IR
H=H/R
HA=H
IF (ER) 433,433,434
433 ER=1.E-11
C433 ER=1.D-11
434 HH=H*H
N1=N
IF (YMIN) 439,440,450
440 YMIN=1.
C440 YMIN=1.D0
439 YMIN= ABS(YMIN)
C439 YMIN=DABS(YMIN)
450 IF (HMAX) 460,460,470
460 HMAX=1.
C460 HMAX=1.D0
470 IF (HMIN) 471,471,472
471 HMIN=1.E-5
C471 HMIN=1.D-5
472 VMIN=ER/(HH*100.)
VMAX=VMIN*100000.
IA=-1
C IA=-1 FOR 1ST (1,2,3 IF R.K.) PASS THRU DAUX
NHH=+1
CALL DAUX
C SAVE INITIAL CONDITIONS FOR RESTART
TZ=T
DO 473 I=1,N1

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DEQ40127
DEQ40128
DEQ40129
DEQ40130
CEQ40131
DEQ40132
DEQ40133
DEQ40134
DEQ40135
DEQ40136
DEQ40137
DEQ40138
DEQ40139
DEQ40140
DEQ40141
DEQ40142
UEQ40143
DEQ40144
DEQ40145
DEQ40146
DEQ40147
DEQ40148
DEQ40149
DEQ40150
DEQ40151
DEQ40152
DEQ40153
DEQ40154
DEQ40155
DEQ40156
DEQ40157
CEQ40158
DEQ40159
DEQ40160
DEQ40161
DEQ40162
DEQ40163
DEQ40164
DEQ40165
DEQ40166
DEQ40167
DEQ40168

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	T5(I)=Y(I)	DEQ40169
	T6(I)=YP(I)	DEQ40170
473	T7(I)=Y2P(I)	DEQ40171
	IF(HMAX-HMIN)261,474,261	DEQ40172
474	NHH=-1	DEQ40173
C	EXIT FROM DEQ2 SETUP	DEQ40174
	GO TO 261	DEQ40175
C	NORMAL INTEGRATION ENTRY. CALL RKCW	DEQ40176
C	ENTRY RKCW	DEQ40177
C	INTEGRATE 1 STEP (H OR H/IR) IN THE COWELL/R.K. MODE	DEQ40178
2	N1=N	DEQ40179
	IF(TEST)900,500,500	DEQ40180
C	R.K. STEP (8R R.K. STEPS)	DEQ40181
500	IDH=1	DEQ40182
501	IF(IKR)505,502,502	DEQ40183
C	R.K. STEP (INITIAL STARTING PROCEDURE)	DEQ40184
502	K=1	DEQ40185
	TEST=TST	DEQ40186
	IKR=-1	DEQ40187
505	GO TO (510,520,530,540,550,560,570,580,590),K	DEQ40188
C	K=1	DEQ40189
510	DO 511 I=1,N1	DEQ40190
	DLT1(I)=Y2P(I)	DEQ40191
	F1P(I)=W0*Y2P(I)	DEQ40192
511	F2P(I)=V0*Y2P(I)	DEQ40193
512	K=K+1	DEQ40194
513	IF(K-10)3,600,3	DEQ40195
C	SPECIAL R.K. INTEGRATION ENTRY. (NTRY=3)	DEQ40196
C	ENTRY RK	DEQ40197
C	INTEGRATE 1 STEP (H, OR H/IR) IN THE RUNGE-KUTTA MODE.	DEQ40198
C	NTRY=3 IS A SPECIAL USAGE. INTEGRATES ONLY IN R.K. MODE	DEQ40199
3	N1=N	DEQ40200
	H1=H	DEQ40201
	HH=H*H	DEQ40202
	H2=H/2.	DEQ40203
	H3=HH/2.	DEQ40204
	H4=H3/2.	DEQ40205
	H5=H4/2.	DEQ40206
	H6=H/6.	DEQ40207
	DO 100 I=1,N1	DEQ40208
	T1(I)=Y(I)	DEQ40209
	T2(I)=YP(I)	DEQ40210

	T3(I)=Y2P(I)	DEQ40211
100	T4(I)=Y2P(I)	DEQ40212
110	T=T+H2	DEQ40213
	IA=-1	DEQ40214
	IF (I)300,200,200	DEQ40215
C	R.K. STEP FOR Y2P=F(X,Y,YP)	DEQ40216
200	DO 210 I=1,N1	DEQ40217
C	Y2P=F(X,Y,YP) IF I1=+	DEQ40218
	Y(I)=T1(I)+H2*T2(I)+H5*Y2P(I)	DEQ40219
210	YP(I)=T2(I)+H2*Y2P(I)	DEQ40220
	CALL DAUX	DEQ40221
	DO 220 I=1,N1	DEQ40222
	T3(I)=T3(I)+Y2P(I)	DEQ40223
	T4(I)=T4(I)+2.*Y2P(I)	DEQ40224
220	YP(I)=T2(I)+H2*Y2P(I)	DEQ40225
	CALL DAUX	DEQ40226
	DO 230 I=1,N1	DEQ40227
	T3(I)=T3(I)+Y2P(I)	DEQ40228
	T4(I)=T4(I)+2.*Y2P(I)	DEQ40229
	Y(I)=T1(I)+H1*T2(I)+H3*Y2P(I)	DEQ40230
230	YP(I)=T2(I)+H1*Y2P(I)	DEQ40231
	T=T+H2	DEQ40232
	CALL DAUX	DEQ40233
	DO 240 I=1,N1	DEQ40234
240	T4(I)=T4(I)+Y2P(I)	DEQ40235
250	DO 260 I=1,N1	DEQ40236
	Y(I)=T1(I)+H1*(T2(I)+H6*T3(I))	DEQ40237
260	YP(I)=T2(I)+H6*(T4(I))	DEQ40238
	IA=+1	DEQ40239
C	IA=+1 FOR FINAL PASS THRU DAUX	DEQ40240
	CALL DAUX	DEQ40241
262	TEST=TEST	DEQ40242
261	RETURN	DEQ40243
C	R.K. STEP FOR Y2P=F(X,Y)	DEQ40244
300	DO 310 I=1,N1	DEQ40245
C	Y2P=F(X,Y) IF I1=-	DEQ40246
310	Y(I)=T1(I)+H2*T2(I)+H5*Y2P(I)	DEQ40247
	CALL DAUX	DEQ40248
	DO 320 I=1,N1	DEQ40249
	T3(I)=T3(I)+2.*Y2P(I)	DEQ40250
320	T4(I)=T4(I)+4.*Y2P(I)	DEQ40251
	T=T+H2	DEQ40252

DO 330 I=1,N1	DEQ40253
330 Y(I)=T1(I)+H1*T2(I)+H3*Y2P(I)	DEQ40254
CALL DAUX	DEQ40255
DO 340 I=1,N1	DEQ40256
340 T4(I)=T4(I)+Y2P(I)	DEQ40257
GO TO 250	DEQ40258
C K=2	DEQ40259
520 DO 521 I=1,N1	DEQ40260
DLT1(I)=DLT1(I)-8.*Y2P(I)	DEQ40261
DLT2(I)=Y2P(I)	DEQ40262
F1P(I)=F1P(I)+W1*Y2P(I)	DEQ40263
521 F2P(I)=F2P(I)+V1*Y2P(I)	DEQ40264
GO TO 512	DEQ40265
C K=3	DEQ40266
530 DO 531 I=1,N1	DEQ40267
DLT1(I)=DLT1(I)+28.*Y2P(I)	DEQ40268
DLT2(I)=7.*Y2P(I)+DLT2(I)	DEQ40269
DLT3(I)=Y2P(I)	DEQ40270
F1P(I)=F1P(I)+W2*Y2P(I)	DEQ40271
531 F2P(I)=F2P(I)+V2*Y2P(I)	DEQ40272
GO TO 512	DEQ40273
C K=4	DEQ40274
540 DO 541 I=1,N1	DEQ40275
DLT1(I)=DLT1(I)-56.*Y2P(I)	DEQ40276
DLT2(I)=DLT2(I)-21.*Y2P(I)	DEQ40277
DLT3(I)=DLT3(I)-6.*Y2P(I)	DEQ40278
DLT4(I)=Y2P(I)	DEQ40279
F1P(I)=F1P(I)+W3*Y2P(I)	DEQ40280
541 F2P(I)=F2P(I)+V3*Y2P(I)	DEQ40281
GO TO 512	DEQ40282
C K=5	DEQ40283
550 DO 551 I=1,N1	DEQ40284
DLT1(I)=DLT1(I)+70.*Y2P(I)	DEQ40285
DLT2(I)=DLT2(I)+35.*Y2P(I)	DEQ40286
DLT3(I)=DLT3(I)+15.*Y2P(I)	DEQ40287
DLT4(I)=5.*Y2P(I)-DLT4(I)	DEQ40288
DLT5(I)=Y2P(I)	DEQ40289
F1P(I)=F1P(I)+W4*Y2P(I)+YP(I)/HA	DEQ40290
551 F2P(I)=F2P(I)+V4*Y2P(I)+(5.*YP(I)/HA)+(Y(I)/(HA*HA))	DEQ40291
GO TO 512	DEQ40292
C K=6	DEQ40293
560 DO 561 I=1,N1	DEQ40294

	DLT1(I)=DLT1(I)-56.*Y2P(I)	DEQ40295
	DLT2(I)=DLT2(I)-35.*Y2P(I)	DEQ40296
	DLT3(I)=DLT3(I)-20.*Y2P(I)	DEQ40297
	DLT4(I)=DLT4(I)-10.*Y2P(I)	DEQ40298
	DLT5(I)=DLT5(I)-4.*Y2P(I)	DEQ40299
	DLT6(I)=Y2P(I)	DEQ40300
	F1P(I)=F1P(I)+W5*Y2P(I)	DEQ40301
561	F2P(I)=F2P(I)+V5*Y2P(I)	DEQ40302
	GO TO 512	DEQ40303
C	K=7	DEQ40304
570	DO 571 I=1,N1	DEQ40305
	DLT1(I)=DLT1(I)+28.*Y2P(I)	DEQ40306
	DLT2(I)=DLT2(I)+21.*Y2P(I)	DEQ40307
	DLT3(I)=DLT3(I)+15.*Y2P(I)	DEQ40308
	DLT4(I)=DLT4(I)+10.*Y2P(I)	DEQ40309
	DLT5(I)=DLT5(I)+6.*Y2P(I)	DEQ40310
	DLT6(I)=3.*Y2P(I)-DLT6(I)	DEQ40311
	DLT7(I)=Y2P(I)	DEQ40312
	F1P(I)=F1P(I)+W6*Y2P(I)	DEQ40313
571	F2P(I)=F2P(I)+V6*Y2P(I)	DEQ40314
	GO TO 512	DEQ40315
C	K=8	DEQ40316
580	DO 581 I=1,N1	DEQ40317
	DLT1(I)=DLT1(I)-8.*Y2P(I)	DEQ40318
	DLT2(I)=DLT2(I)-7.*Y2P(I)	DEQ40319
	DLT3(I)=DLT3(I)-6.*Y2P(I)	DEQ40320
	DLT4(I)=DLT4(I)-5.*Y2P(I)	DEQ40321
	DLT5(I)=DLT5(I)-4.*Y2P(I)	DEQ40322
	DLT6(I)=DLT6(I)-3.*Y2P(I)	DEQ40323
	DLT7(I)=DLT7(I)-2.*Y2P(I)	DEQ40324
	DLT8(I)=Y2P(I)	DEQ40325
	F1P(I)=F1P(I)+W7*Y2P(I)	DEQ40326
581	F2P(I)=F2P(I)+V7*Y2P(I)	DEQ40327
	GO TO 512	DEQ40328
C	K=9	DEQ40329
590	DO 591 I=1,N1	DEQ40330
	DLT1(I)=DLT1(I)+Y2P(I)	DEQ40331
	DLT2(I)=DLT2(I)+Y2P(I)	DEQ40332
	DLT3(I)=DLT3(I)+Y2P(I)	DEQ40333
	DLT4(I)=DLT4(I)+Y2P(I)	DEQ40334
	DLT5(I)=DLT5(I)+Y2P(I)	DEQ40335
	DLT6(I)=DLT6(I)+Y2P(I)	DEQ40336

DLT7(I)=DLT7(I)+Y2P(I)	DEQ40337
DLT8(I)=Y2P(I)-DLT8(I)	DEQ40338
F1P(I)=F1P(I)+W8*Y2P(I)	DEQ40339
591 F2P(I)=F2P(I)+V8*Y2P(I)	DEQ40340
GO TO 512	DEQ40341
C ENTRY CW	DEQ40342
600 K=1	DEQ40343
KC=1	DEQ40344
KS=1	DEQ40345
RAT=1.	DEQ40346
NDUB=+1	DEQ40347
NH2=NHH	DEQ40348
NVR=1	DEQ40349
NJH3=+1	DEQ40350
C TEST FOR HALVING AND DOUBLING	DEQ40351
C IDH=1 IF STEP=SIZE HAS NOT CHANGED.	DEQ40352
900 IDH=1	DEQ40353
IC=IB+1	DEQ40354
IF (I2)1000,901,901	DEQ40355
901 IF(NH2)9011,9010,9010	DEQ40356
9010 DO 902 I=1,IB	DEQ40357
IF(ABS(DLT2(I)/AMAX1(ABS(Y(I)),YMIN)).GE.VMAX) GO TO 1100	DEQ40358
C IF(DABS(DLT2(I)/DMAX1(DABS(Y(I)),YMIN)).GE.VMAX) GO TO 1100	DEQ40359
902 CONTINUE	DEQ40360
C IF 2.*H G.T. HMAX, STOP DOUBLING TEST	DEQ40361
9011 IF(NDUB)980,9020,9020	DEQ40362
9020 IF(NVR)980,980,9021	DEQ40363
9021 IF(RAT=1.)9022,9022,980	DEQ40364
9022 IF(KS)954,954,9023	DEQ40365
9023 DO 903 I=1,IB	DEQ40366
IF(ABS(DLT2(I)/AMAX1(ABS(Y(I)),YMIN)).GE.VMIN) GO TO 980	DEQ40367
C IF(DABS(DLT2(I)/DMAX1(DABS(Y(I)),YMIN)).GE.VMIN) GO TO 980	DEQ40368
903 CONTINUE	DEQ40369
C TEST FURTHER FOR DOUBLING.	DEQ40370
DO 904 I=1,IB	DEQ40371
IF(ABS(DLT1(I)/AMAX1(ABS(Y(I)),YMIN)).GE.VMIN) GO TO 980	DEQ40372
C IF(DABS(DLT1(I)/DMAX1(DABS(Y(I)),YMIN)).GE.VMIN) GO TO 980	DEQ40373
904 CONTINUE	DEQ40374
C IF HERE, CURRENT STEP O.K. FOR DOUBLING.	DEQ40375
950 TMP4=H+H	DEQ40376
IF(ABS(TMP4).GT.HMAX) GO TO 3000	DEQ40377
C IF(DABS(TMP4).GT.HMAX) GO TO 3000	DEQ40378

C	KJ=1 (SAVE ALL EQUATIONS FOR DOUBLING)	DEQ40379
	KJ=1	DEQ40380
952	KA=KC	DEQ40381
	KC=KC+1	DEQ40382
	GO TO (2010,2020,2030,2040,2050,2060,2070,2080,2090),KA	DEQ40383
954	KS=-KS	DEQ40384
	GO TO 1000	DEQ40385
980	IF (IB=N1) 981,3002,981	DEQ40386
981	IF (RXH-1.) 3002,3002,990	DEQ40387
990	IF (KS) 954,954,992	DEQ40388
992	KJ=IB+1	DEQ40389
	VAR=VARX*VMIN/RAT	DEQ40390
	DO 991 I=KJ,N1	DEQ40391
	IF (ABS(DLT2(I)/AMAX1(ABS(Y(I)),YMIN)).GE.VAR) GO TO 3002	DEQ40392
991	CONTINUE	DEQ40393
	NVR=-1	DEQ40394
	GO TO 952	DEQ40395
C	HALVE H; RETURN TO R.K.	DEQ40396
1100	R=IR	DEQ40397
	H=H/(2.*R)	DEQ40398
	IF (ABS(H).LT.HMIN) GO TO 3050	DEQ40399
C	IF (DARS(H).LT.HMIN) GO TO 3050	DEQ40400
	IDH=2	DEQ40401
	RXH=RXA	DEQ40402
	TST=+1.	DEQ40403
	TEST=3.	DEQ40404
	IF (NJH3) 1104,1101,1101	DEQ40405
1101	IF (NSTRT) 1102,1106,1106	DEQ40406
1102	TEST=2.	DEQ40407
C	RESTORE INITIAL CONDITIONS AND RESTART. (TEST=2.)	DEQ40408
1104	T=TZ	DEQ40409
	TST=TEST	DEQ40410
	DO 1105 I=1,N1	DEQ40411
	Y(I)=T5(I)	DEQ40412
	YP(I)=T6(I)	DEQ40413
1105	Y2P(I)=T7(I)	DEQ40414
1106	IKR=+1	DEQ40415
	HA=H	DEQ40416
	VMIN=ER/(H*H*100.)	DEQ40417
	VMAX=VMIN*100000.	DEQ40418
	GO TO 502	DEQ40419
C	KA=1 SAVE Y2P(0) IN T2 (ACCUM, F1P(2H), F2P(2H))	DEQ40420

2010	DO 2011 I=KJ,N1	DEQ40421
	T2(I)=Y2P(I)	DEQ40422
	T6(I)=W0*Y2P(I)	DEQ40423
2011	T7(I)=V0*Y2P(I)	DEQ40424
	GO TO 954	DEQ40425
C	K1=2 SAVE Y2P(2) IN T3 (ACCUM. F1P(2H), F2P(2H))	DEQ40426
2020	DO 2021 I=KJ,N1	DEQ40427
	T3(I)=Y2P(I)	DEQ40428
	T6(I)=T6(I)+W1*Y2P(I)	DEQ40429
2021	T7(I)=T7(I)+V1*Y2P(I)	DEQ40430
	GO TO 954	DEQ40431
C	K1=3 SAVE Y2P(4) IN T4 (ACCUM. F1P(2H), F2P(2H))	DEQ40432
2030	DO 2031 I=KJ,N1	DEQ40433
	T4(I)=Y2P(I)	DEQ40434
	T6(I)=T6(I)+W2*Y2P(I)	DEQ40435
2031	T7(I)=T7(I)+V2*Y2P(I)	DEQ40436
	GO TO 954	DEQ40437
C	K1=4 SAVE Y2P(6) IN T5 (ACCUM. F1P(2H), F2P(2H))	DEQ40438
2040	DO 2041 I=KJ,N1	DEQ40439
	T5(I)=Y2P(I)	DEQ40440
	T6(I)=T6(I)+W3*Y2P(I)	DEQ40441
2041	T7(I)=T7(I)+V3*Y2P(I)	DEQ40442
	GO TO 954	DEQ40443
C	K1=5 (ACCUM. F1P(2H), F2P(2H) FOR DOUBLING)	DEQ40444
2050	H1=1./(H+H)	DEQ40445
	H2=H1*H1	DEQ40446
	H3=1./RAT	DEQ40447
	H4=H3*H3	DEQ40448
	DO 2051 I=KJ,N1	DEQ40449
	IF(I-IC)2053,2052,2053	DEQ40450
2052	H1=H1*H3	DEQ40451
	H2=H2*H4	DEQ40452
2053	T6(I)=T6(I)+W4*Y2P(I)+YP(I)*H1	DEQ40453
2051	T7(I)=T7(I)+V4*Y2P(I)+5.*YP(I)*H1+Y(I)*H2	DEQ40454
	GO TO 954	DEQ40455
C	K1=6 (ACCUM. F1P(2H), F2P(2H) FOR DOUBLING)	DEQ40456
2060	DO 2061 I=KJ,N1	DEQ40457
	T6(I)=T6(I)+W5*Y2P(I)	DEQ40458
2061	T7(I)=T7(I)+V5*Y2P(I)	DEQ40459
	GO TO 954	DEQ40460
C	K1=7 (ACCUM. F1P(2H), F2P(2H) FOR DOUBLING)	DEQ40461
2070	DO 2071 I=KJ,N1	DEQ40462

	T6(I)=T6(I)+W6*Y2P(I)	DEQ40463
2071	T7(I)=T7(I)+V6*Y2P(I)	DEQ40464
	GO TO 954	DEQ40465
C	K1=8 (ACCUM. F1P(2H), F2P(2H) FOR DOUBLING)	DEQ40466
2080	DO 2081 I=KJ,N1	DEQ40467
	T6(I)=T6(I)+W7*Y2P(I)	DEQ40468
2081	T7(I)=T7(I)+V7*Y2P(I)	DEQ40469
	GO TO 954	DEQ40470
C	K1=9 (ACCUM. F1P(2H), F2P(2H) FOR DOUBLING)	DEQ40471
2090	DO 2091 I=KJ,N1	DEQ40472
	F1P(I)=T6(I)+W8*Y2P(I)	DEQ40473
	F2P(I)=T7(I)+V8*Y2P(I)	DEQ40474
C	DOUBLE H IN COWELL MODE	DEQ40475
	DLT8(I)= 2.*DLT8(I)-DLT7(I)	DEQ40476
	DLT7(I)= 4.*DLT7(I)-(4.*DLT6(I)-DLT5(I))	DEQ40477
	DLT6(I)= 8.*DLT6(I)-(12.*DLT5(I)-6.*DLT4(I)+DLT3(I))	DEQ40478
	DLT5(I)=16.*DLT5(I)-(32.*DLT4(I)-24.*DLT3(I)+8.*DLT2(I)-DLT1(I))	DEQ40479
	DLT4(I)= 5.*DLT5(I)-(10.*DLT6(I)-10.*DLT7(I)+5.*DLT8(I))	DEQ40480
	1+(Y2P(I)-T5(I))	DEQ40481
	DLT3(I)= 6.*DLT4(I)-(15.*DLT5(I)-20.*DLT6(I)+15.*DLT7(I)	DEQ40482
	1-6.*DLT8(I))-(Y2P(I)-T4(I))	DEQ40483
	DLT2(I)= 7.*DLT3(I)-(21.*DLT4(I)-35.*DLT5(I)+35.*DLT6(I)	DEQ40484
	1-21.*DLT7(I)+7.*DLT8(I))+(Y2P(I)-T3(I))	DEQ40485
	DLT1(I)= 8.*DLT2(I)-(28.*DLT3(I)-56.*DLT4(I)+70.*DLT5(I)	DEQ40486
	1-56.*DLT6(I)+28.*DLT7(I)-8.*DLT8(I))-(Y2P(I)-T2(I))	DEQ40487
2091	CONTINUE	DEQ40488
C	END OF DOUBLING	DEQ40489
	IF(NVR)2093,2092,2092	DEQ40490
2092	IDH=3	DEQ40491
	VMIN=VMIN/4.	DEQ40492
	VMAX=VMAX/4.	DEQ40493
	H=H+H	DEQ40494
	HA=H	DEQ40495
	NH2=NH	DEQ40496
	GO TO 2095	DEQ40497
3000	NDUB=-1	DEQ40498
3002	NJH3=+1	DEQ40499
	IF(NH2)2095,3004,3004	DEQ40500
3004	IF(JHH-3)2095,3006,2095	DEQ40501
3006	NJH3=-1	DEQ40502
	TZ=T	DEQ40503
	DO 3010 I=1,N1	DEQ40504

T5(I)=Y(I)	DEQ40505
T6(I)=YP(I)	DEQ40506
3010 T7(I)=Y2P(I)	DEQ40507
GO TO 2095	DEQ40508
3050 NH2=-1	DEQ40509
IF(NSTRT)3052,1000,1000	DEQ40510
3052 TEST=13.	DEQ40511
GO TO 261	DEQ40512
2093 RAT=2.*RAT	DEQ40513
K=K+K	DEQ40514
RKH=KKH-1.	DEQ40515
IDH=4	DEQ40516
2095 KC=1	DEQ40517
KS=1	DEQ40518
C STEP-SIZE O.K., PROCEED WITH COWELL STEP.	DEQ40519
1000 TEST=-1.	DEQ40520
H=HA	DEQ40521
NSTRT=+1	DEQ40522
HH=H*H	DEQ40523
NX=IB	DEQ40524
C COMPLETE K STEPS FOR FIRST 18 EQNS.	DEQ40525
DO 1022 K1=1,K	DEQ40526
T=T+H	DEQ40527
IF(K-K1)6660,6660,6661	DEQ40528
6660 NX=N1	DEQ40529
TEST=+1.	DEQ40530
6661 DO 1001 I=1,NX	DEQ40531
IF(I-IC)6666,6665,6666	DEQ40532
6665 H=HA*RAT	DEQ40533
HH=H*H	DEQ40534
6666 T1(I)=Y2P(I)	DEQ40535
1001 Y(I) =HH*(F2P(I)+A0*Y2P(I)+A1*DLT8(I)+A2*DLT7(I)+A3*DLT6(I)	DEQ40536
1 +A4*DLT5(I)+A5*DLT4(I)+A6*DLT3(I)+A7*DLT2(I)+A8*DLT1(I))	DEQ40537
H=HA	DEQ40538
IF(I1)1007,1005,1005	DEQ40539
1005 DO 1006 I=1,NX	DEQ40540
IF(I-IC)1006,6667,1006	DEQ40541
6667 H=HA*RAT	DEQ40542
1006 YP(I)=H*(F1P(I)+AP0*Y2P(I)+AP1*DLT8(I)+AP2*DLT7(I)+AP3*DLT6(I)	DEQ40543
1 +AP4*DLT5(I)+AP5*DLT4(I)+AP6*DLT3(I)+AP7*DLT2(I)+AP8*DLT1(I))	DEQ40544
1007 ASSIGN 1015 TO IFLAG	DEQ40545
IA=-1	DEQ40546

1010	CALL DAUX	DEQ40547
	H=HA	DEQ40548
	HH=H*H	DEQ40549
1009	DO 1013 I=1,NX	DEQ40550
	IF(I-IC)6669,6668,6669	DEQ40551
6668	H=HA*RAI	DEQ40552
	HH=H*H	DEQ40553
6669	TMP1=Y2P(I)-T1(I)	DEQ40554
	TMP2=TMP1-DLT8(I)	DEQ40555
	TMP3=TMP2-DLT7(I)	DEQ40556
	TMP4=TMP3-DLT6(I)	DEQ40557
	TMP5=TMP4-DLT5(I)	DEQ40558
	TMP6=TMP5-DLT4(I)	DEQ40559
	TMP7=TMP6-DLT3(I)	DEQ40560
	TMP8=TMP7-DLT2(I)	DEQ40561
	Y(I)=HH*(F2P(I)+HA*Y2P(I)+B1*TMP1+B2*TMP2+B3*TMP3+B4*TMP4+B5*TMP5	DEQ40562
	+B6*TMP6+B7*TMP7+B8*TMP8)	DEQ40563
1011	YP(I)=H*(F1P(I)+BP0*Y2P(I)+BP1*TMP1+BP2*TMP2+BP3*TMP3+BP4*TMP4	DEQ40564
	+BP5*TMP5+BP6*TMP6+BP7*TMP7+BP8*TMP8)	DEQ40565
1013	CONTINUE	DEQ40566
	GO TO IFLAG*(1015,1020)	DEQ40567
1015	ASSIGN 1020 TO IFLAG	DEQ40568
	IA=+1	DEQ40569
	GO TO 1010	DEQ40570
1020	DO 1021 I=1,NX	DEQ40571
	TMP1=Y2P(I)-T1(I)	DEQ40572
	TMP2=TMP1-DLT8(I)	DEQ40573
	DLT8(I)=TMP1	DEQ40574
	TMP1=TMP2-DLT7(I)	DEQ40575
	DLT7(I)=TMP2	DEQ40576
	TMP2=TMP1-DLT6(I)	DEQ40577
	DLT6(I)=TMP1	DEQ40578
	TMP1=TMP2-DLT5(I)	DEQ40579
	DLT5(I)=TMP2	DEQ40580
	TMP2=TMP1-DLT4(I)	DEQ40581
	DLT4(I)=TMP1	DEQ40582
	TMP1=TMP2-DLT3(I)	DEQ40583
	DLT3(I)=TMP2	DEQ40584
	DLT1(I)=TMP1-DLT2(I)	DEQ40585
	DLT2(I)=TMP1	DEQ40586
	F1P(I)=F1P(I)+Y2P(I)	DEQ40587
1021	F2P(I)=F2P(I)+F1P(I)	DEQ40588

TEST=TFST-1.
H=HA
HH=HA*HA
1022 CONTINUE
TEST=-1.
GO TO 201
END

DEQ40589
UEQ40590
DEQ40591
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13 ABSTRACT ASC DEQ4 is a floating point subroutine, written in FORTRAN IV source language, which integrates numerically a set of N simultaneous second-order ordinary differential equations in which first derivatives may or may not appear [i.e., $y_i'' = f(t, y_i, y_i')$ or $y_i'' = f(t, y_i)$, $i = 1, 2, \dots, N$]. If the N equations can be separated into two groups (IB and N-IB) such that the first IB equations are not dependent on the final N-IB equations (e.g., variational equations) then DEQ4 has the capability of integrating the final N-IB equations at a larger step size than the first IB equations, thus saving $2(R-1)(N-IB)$ derivatives per integration step. This subroutine obsoletes subroutine DEQ2 with the following improvements: better accuracy controls, new starting procedure, improved halving and doubling procedure, reduction in computing time, and reduction in core storage requirements (10N less). The subroutine is restricted in that it contains 20 digit octal constants (real constants) for the CDC 6000 series machines.		

Floating Point Cowell (Second-Sum)
Runge-Kutta Integration
Second-Order Ordinary Differential Equations
Two-Group Multi-Step Mode
Subroutine
Step Size

Abstract (Continued)